Methallyl alcohol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.27 days

Global applicability domain: Outside

Local applicability domain index: 3.70e-01

Confidence level: 7.69e-01

Nearest Neighbors from the Training Set

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Propylbenzene
Measured: 24.3
Predicted: 4.02

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Tetradeca-1,13-diene
Measured: 367
Predicted: 8.69

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2-Methylhexane
Measured: 12.5
Predicted: 5.54

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2-Methylheptane
Measured: 12.5
Predicted: 3.99